

N-Butyl-3-chloro-6-hydrazinylpyridazin-4-amine
61261-46-9 | DTXSID90615440

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 188 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.80e-01

Confidence level: 8.59e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Atrazine</div> <div>Measured: 174</div> <div>Predicted: 202</div>	<div>Image not found</div> <div>Simazine</div> <div>Measured: 126</div> <div>Predicted: 135</div>	<div>Image not found</div> <div>Phenazopyridine</div> <div>Measured: 209</div> <div>Predicted: 268</div>
<div>Image not found</div> <div>Simetone</div> <div>Measured: 219</div> <div>Predicted: 218</div>	<div>Image not found</div> <div>Propazine</div> <div>Measured: 251</div> <div>Predicted: 280</div>	